Stress Relaxation Due to Dislocation Formation in Orthorhombic Ga_2O_3 Films Grown on Al_2O_3 Substrates

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Abstract

We analyze the preference of various types of misfit dislocation (MD) formation in film/substrate κ-Ga_2O_3/α-Al_2O_3 and κ-$(Al_xGa_{1-x})_2O_3$/κ-Al_2O_3 heterostructures. We consider two possibilities for variation in films growth orientation (defined by inclination angle ϑ) for these heterostructures with inclination axes about either [100] or [010] crystallographic directions. We study dependences of the critical film thickness for MD formation on the inclination angle ϑ for heterostructures under consideration. We find the presence of two special orientations (ϑ ~ 26° for [100] heterostructure, ϑ ~ 28° for [010] heterostructure, and ϑ = 90° for both inclination types) of κ-Ga_2O_3/α-Al_2O_3 heterostructures, for which the formation of MDs is energetically unfavorable. We show that formation of pure edge MDs is easier for [010] κ-$(Al_xGa_{1-x})_2O_3$/κ-Al_2O_3 heterostructures than for [100] heterostructures, and it is vice versa for mixed MDs in these heterostructures.

Keywords: Film/substrate heterostructures; Gallium oxide; Growth orientation; Misfit dislocations

1. INTRODUCTION

Gallium oxide (Ga_2O_3), one of the ultra-wide bandgap semiconductors, has attracted much attention in recent years due to great prospects in power electronic devices including those for space and nuclear industries, photoelectric converters for the ultraviolet region, high-power radio frequency devices, gas sensors, etc. [1–3]. An important feature of Ga_2O_3 is the possibility of its existence in various polymorphic forms: stable monoclinic β-phase, and metastable α-, γ-, κ-, ε- and δ-phases with their specific characteristics and benefits [4–8]. The metastable hexagonal ε-Ga_2O_3 is of particular interest due to its favorable growth features and great compatibility with common substrates and the possibility of polarization engineering endowed by its polar nature [9]. Early reports investigated a hexagonal $P6_3mc$ structure for ε-Ga_2O_3, while recent investigations identified its orthorhombic structure in the $Pna2_1$ symmetry group, denoted as κ-Ga_2O_3 [10,11]. The pseudohexagonal structure of ε-phase consists of 120° rotational orthorhombic κ-Ga_2O_3 domains. However, until now, some works indicate the possibility of the existence of pure ε-phase [12]. Despite the ongoing debate about the real structure of the considered phase, most scientific groups tend to consider the phase as composed of 3-fold rotational orthorhombic domains with disordered domain boundaries [10,11,13,14]; the single-domain orthorhombic structure of this phase has been recently demonstrated [3,15]. Therefore, in this work, we will consider this phase as κ-Ga_2O_3 with the orthorhombic crystal structure $Pna2_1$.

The heterostructures based on κ-Ga_2O_3 are successfully used in solar blind photodetectors [16], powerful Schottky diodes [17], and in high-frequency applications [18]. Unfortunately, the characteristics of these devices are limited by the crystal quality of the κ-Ga_2O_3 film/layer/heterostructures, which are characterized by a high dislocation density that ranges from 5.2×10^7 to 1.4×10^{13} cm^{-2} [3,19]. Such a wide scatter in the value of the dislocation density can be due to the insufficient

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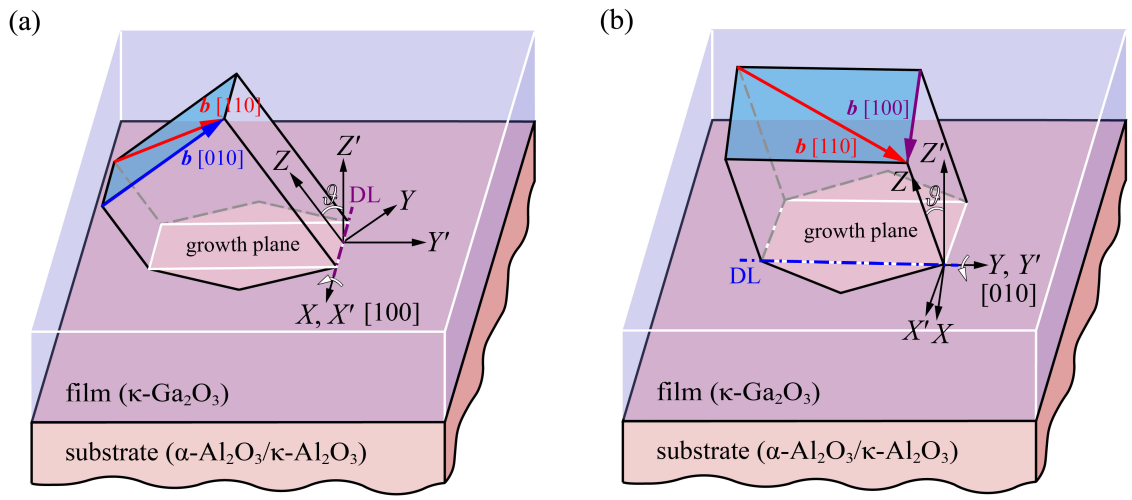

Fig. 1. Schematics of the film/substrate heterostructure with selected coordinate systems that are used in the calculations. Frame (a) shows heterostructure with inclination axis about [100] crystallographic direction for κ-Ga_2O_3/κ-Al_2O_3 (i.e., about $[2\bar{1}\bar{1}0]$ for α-Al_2O_3); frame (b) shows heterostructure with inclination axis about [010] crystallographic direction for κ-Ga_2O_3/κ-Al_2O_3 (i.e., about $[\bar{1}2\bar{1}0]$ for α-Al_2O_3). ϑ is the angle between the *c*-axis (Z-axis) of κ-Ga_2O_3 and the normal one to the film plane (Z′-axis). Blue surfaces show (001) crystallographic plane of κ-Ga_2O_3. Red, blue and purple arrows show the direction of Burgers vector ***b*** along [110], [010] and [100] crystallographic directions, respectively. Dash-dotted lines indicate dislocation lines (DLs).

knowledge on the optimal parameters of the heterostructure, including substrate material, crystallographic orientation of the substrate, film thickness, etc. in order to grow κ-Ga_2O_3 with the minimum possible number of defects. In this work, we propose a theoretical model that allows to find the critical conditions of the system for the formation of misfit dislocations (MDs) in κ-Ga_2O_3/α-Al_2O_3 and κ-$(Al_xGa_{1-x})_2O_3$/κ-Al_2O_3 heterostructures.

2. MODEL

Similarly to the approach described in Refs. [20–25], we consider a film/substrate κ-Ga_2O_3/Al_2O_3 heterostructure with thin film and MDs formed at the interface (Fig. 1). Since the film consists of the κ-Ga_2O_3, it is possible to assume the following variation in heterostructure growth orientations with minimal mismatch between κ-Ga_2O_3 film and α-Al_2O_3 or κ-Al_2O_3 substrate: (i) heterostructure with inclination axes about $\langle 100 \rangle$-type crystallographic directions for κ-Ga_2O_3/κ-Al_2O_3 (i.e. about $\langle 2\bar{1}\bar{1}0 \rangle$ for α-Al_2O_3), see Fig. 1a, and (ii) heterostructure with inclination axes about $\langle 010 \rangle$-type crystallographic directions for κ-Ga_2O_3/κ-Al_2O_3 (i.e. about $\langle \bar{1}100 \rangle$ for α-Al_2O_3), see Fig. 1b. The inclination angle is given as ϑ in Fig. 1.

In general, the MDs formed at the heterointerface as a result of stress relaxation process are mixed dislocations, which have both edge and screw Burgers vector components. The Burgers vectors (colored arrows) and dislocation lines (DLs; colored dash-dotted lines) of such MDs are shown in Fig. 1. Red, blue and purple arrows correspond to Burgers vector along [111], [010] and [100] crystallographic directions, respectively; DLs are parallel to inclination axes. In this work, we consider only mixed and pure edge MDs; pure screw MDs do not contribute to the misfit stresses relaxation in the case of a biaxial stress-strain state under consideration [26].

Our model, which describes the critical conditions for the MDs formation in κ-Ga_2O_3/α-Al_2O_3 and κ-Ga_2O_3/κ-Al_2O_3 heterostructures, is based on the Matthews-Blakeslee (M-B) approach [27,28]. For the elastically semi-isotropic case, the M-B approach gives the simplified expression for finding the critical thickness h_c for MD formation [20]:

$$h_c = \frac{b_{\parallel}^2 + b_{\perp}^2 + (1-\nu) b_s^2}{\varepsilon_m (1+\nu) 8\pi b_{\parallel}} \ln\left(\frac{2h_c}{r_0}\right), \quad (1)$$

where ε_m is the component of the lattice mismatch released by MDs; ν is Poisson ratio (ν = 0.3 in our calculations); $b_{\parallel}$ and $b_{\perp}$ are the projections of the edge component of the dislocation Burgers vector parallel and perpendicular heterointerface, respectively, and b_s is the magnitude of the screw component of the dislocation Burgers vector; r_0 is the dislocation core radius parameter. The magnitude of the Burgers vector ***b*** is related to the components: $b^2 = b_{\parallel}^2 + b_{\perp}^2 + b_s^2$.

The anisotropy of the film and substrate materials is considered in the parameter ε_m, which takes the following form:

$$\varepsilon_m = \frac{a_{\alpha\text{-}Al_2O_3}\sqrt{3}c_{\alpha\text{-}Al_2O_3} - \sqrt{(b_{\kappa\text{-}Ga_2O_3}c_{\alpha\text{-}Al_2O_3})^2\cos^2\vartheta + 3(a_{\alpha\text{-}Al_2O_3}c_{\kappa\text{-}Ga_2O_3})^2\sin^2\vartheta}}{\sqrt{(b_{\kappa\text{-}Ga_2O_3}c_{\alpha\text{-}Al_2O_3})^2\cos^2\vartheta + 3(a_{\alpha\text{-}Al_2O_3}c_{\kappa\text{-}Ga_2O_3})^2\sin^2\vartheta}} \quad (2)$$

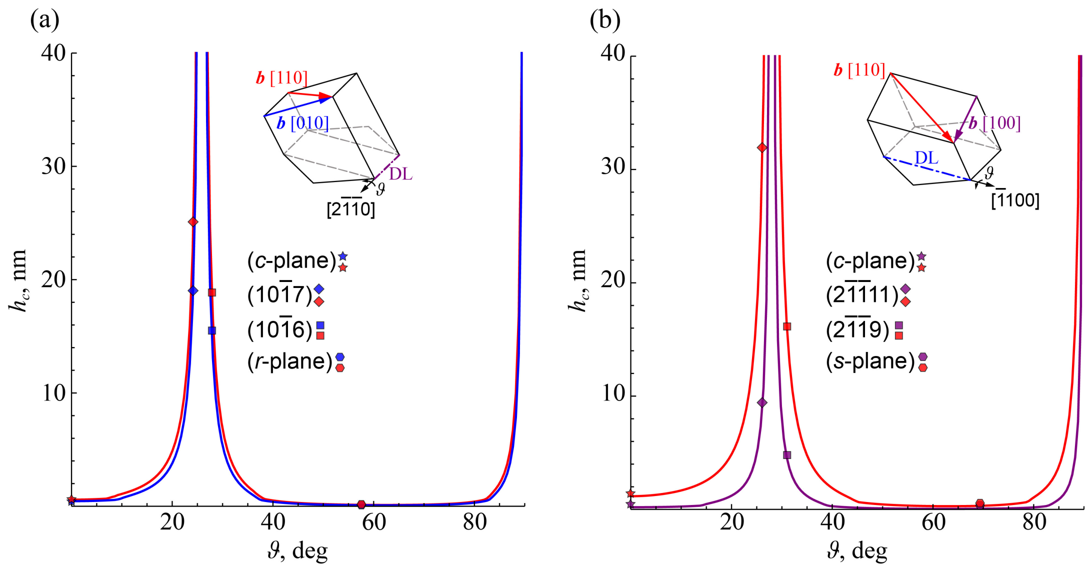

Fig. 2. Dependences of the critical thickness h_c on the inclination angle ϑ for κ-Ga_2O_3/α-Al_2O_3 heterostructures. Frames (a) and (b) show dependences for heterostructures with inclination axes about $[2\bar{1}\bar{1}0]$ and $[\bar{1}100]$ crystallographic direction of α-Al_2O_3 substrate, respectively. Red, blue and purple curves describe the cases of MDs with Burgers vector ***b*** along [110], [010] and [100] crystallographic directions, respectively. Bullets indicate h_c values for various growth planes of the α-Al_2O_3 substrate.

for κ-Ga_2O_3/α-Al_2O_3 heterostructure with inclination axis about [100] crystallographic direction of the film or $[2\bar{1}\bar{1}0]$ crystallographic direction of the substrate;

$$\varepsilon_m = \frac{a_{\alpha\text{-}Al_2O_3} c_{\alpha\text{-}Al_2O_3} - \sqrt{(a_{\kappa\text{-}Ga_2O_3} c_{\alpha\text{-}Al_2O_3})^2 \cos^2\vartheta + (a_{\alpha\text{-}Al_2O_3} c_{\kappa\text{-}Ga_2O_3})^2 \sin^2\vartheta}}{\sqrt{(a_{\kappa\text{-}Ga_2O_3} c_{\alpha\text{-}Al_2O_3})^2 \cos^2\vartheta + (a_{\alpha\text{-}Al_2O_3} c_{\kappa\text{-}Ga_2O_3})^2 \sin^2\vartheta}}, \tag{3}$$

for heterostructure κ-Ga_2O_3/α-Al_2O_3 with inclination axis about [010] crystallographic direction of the film or $[\bar{1}100]$ crystallographic direction of the substrate;

$$\varepsilon_m = \frac{b_{\kappa\text{-}Al_2O_3} c_{\kappa\text{-}Al_2O_3} - \sqrt{(b_{\kappa\text{-}Ga_2O_3} c_{\kappa\text{-}Al_2O_3})^2 \cos^2\vartheta + (b_{\kappa\text{-}Al_2O_3} c_{\kappa\text{-}Ga_2O_3})^2 \sin^2\vartheta}}{\sqrt{(b_{\kappa\text{-}Ga_2O_3} c_{\kappa\text{-}Al_2O_3})^2 \cos^2\vartheta + 3(b_{\kappa\text{-}Al_2O_3} c_{\kappa\text{-}Ga_2O_3})^2 \sin^2\vartheta}}, \tag{4}$$

for κ-Ga_2O_3/κ-Al_2O_3 heterostructure with inclination axis about [100] crystallographic direction;

$$\varepsilon_m = \frac{a_{\kappa\text{-}Al_2O_3} c_{\kappa\text{-}Al_2O_3} - \sqrt{(a_{\kappa\text{-}Ga_2O_3} c_{\kappa\text{-}Al_2O_3})^2 \cos^2\vartheta + (a_{\kappa\text{-}Al_2O_3} c_{\kappa\text{-}Ga_2O_3})^2 \sin^2\vartheta}}{\sqrt{(a_{\kappa\text{-}Ga_2O_3} c_{\kappa\text{-}Al_2O_3})^2 \cos^2\vartheta + (a_{\kappa\text{-}Al_2O_3} c_{\kappa\text{-}Ga_2O_3})^2 \sin^2\vartheta}}, \tag{5}$$

for heterostructure κ-Ga_2O_3/κ-Al_2O_3 with inclination axis about [010] crystallographic direction $a_{\kappa\text{-}Ga_2O_3}$, $b_{\kappa\text{-}Ga_2O_3}$, $c_{\kappa\text{-}Ga_2O_3}$, $a_{\alpha\text{-}Al_2O_3}$, $c_{\alpha\text{-}Al_2O_3}$, $a_{\kappa\text{-}Al_2O_3}$, $b_{\kappa\text{-}Al_2O_3}$, $c_{\kappa\text{-}Al_2O_3}$ are the crystal lattice parameters of κ-Ga_2O_3, α-Al_2O_3 and κ-Al_2O_3; their values are given in Table 1.

The possible orientations of the Burgers vector are chosen based on the crystal structure of κ-Ga_2O_3 such as parallel to [100], [010] and [110] crystallographic directions. In the case of the heterostructures with inclination axis [100], the projections of the Burgers vector have the form:

$$\boldsymbol{b}\,[100]\text{:}\ b_s = a_{\kappa\text{-}Ga_2O_3},\ b_\parallel = 0,\ b_\perp = 0,$$

$$\boldsymbol{b}\,[010]\text{:}\ b_s = 0,\ b_\parallel = b_{\kappa\text{-}Ga_2O_3}\cos\vartheta,\ b_\perp = b_{\kappa\text{-}Ga_2O_3}\sin\vartheta,$$

$$\boldsymbol{b}\,[110]\text{:}\ b_s = a_{\kappa\text{-}Ga_2O_3},\ b_\parallel = b_{\kappa\text{-}Ga_2O_3}\cos\vartheta,\ b_\perp = b_{\kappa\text{-}Ga_2O_3}\sin\vartheta, \tag{6}$$

and in the case of the heterostructures with inclination axis [010], the projections of the Burgers vector have the form:

$$\boldsymbol{b}\,[100]\text{:}\ b_s = 0,\ b_\parallel = a_{\kappa\text{-}Ga_2O_3}\cos\vartheta,\ b_\perp = -a_{\kappa\text{-}Ga_2O_3}\sin\vartheta,$$

$$\boldsymbol{b}\,[010]\text{:}\ b_s = b_{\kappa\text{-}Ga_2O_3},\ b_\parallel = 0,\ b_\perp = 0,$$

$$\boldsymbol{b}\,[110]\text{:}\ b_s = b_{\kappa\text{-}Ga_2O_3},\ b_\parallel = a_{\kappa\text{-}Ga_2O_3}\cos\vartheta,\ b_\perp = -a_{\kappa\text{-}Ga_2O_3}\sin\vartheta. \tag{7}$$

3. RESULTS AND DISCUSSION

Figure 2 presents the calculated dependences of the critical film thickness h_c for the formation of various types of MDs on the inclination angle ϑ for κ-Ga_2O_3/α-Al_2O_3 heterostructures. A feature of these dependences is the

Table 1. Crystal lattice parameters of materials under consideration.

Lattice parameters (Å)	κ-Ga_2O_3 [29] $Pna2_1$	α-Al_2O_3 [30] $R\bar{3}c:H$	κ-Al_2O_3 [29] $Pna2_1$
a	5.078	4.761	4.848
b	8.706	4.761	8.323
c	9.308	12.996	8.944

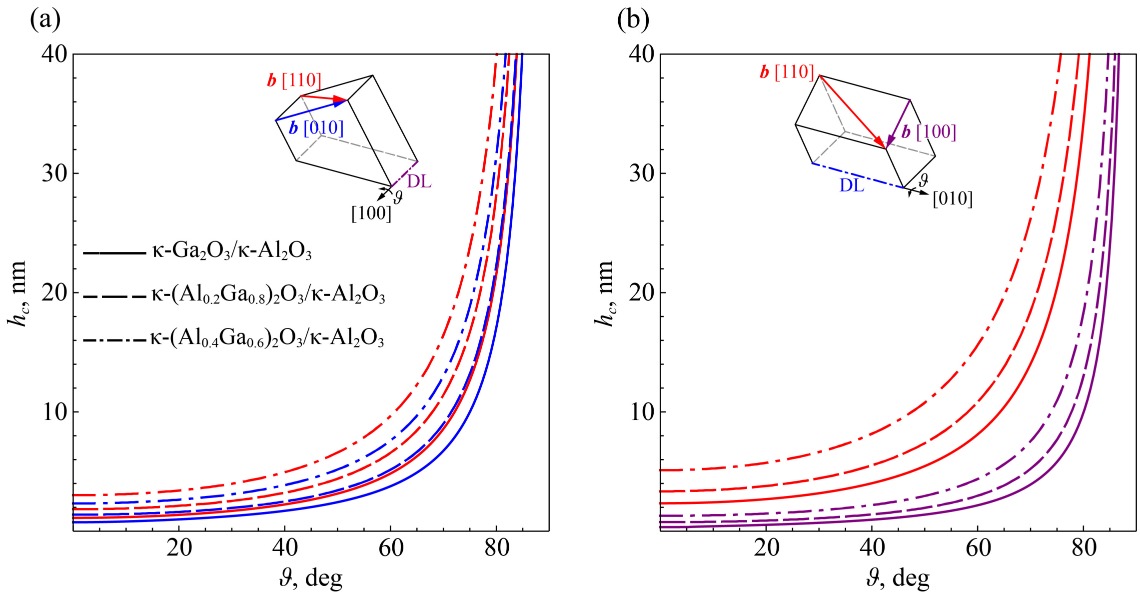

Fig. 3. Dependences of the critical thickness h_c on the inclination angle ϑ for κ-$(Al_xGa_{1-x})_2O_3$/κ-Al_2O_3 heterostructures. Frames (a) and (b) show dependences for heterostructures with inclination axes about [100] and [010] crystallographic direction of κ-Al_2O_3 substrate, respectively. Solid, dashed and dash-dotted curves correspond to the value of Al composition $x = 0$, 0.2, and 0.4 respectively.

presence of two special orientations of heterostructures in which the formation of MDs is energetically unfavorable. First special case takes place at $\vartheta \sim 26°$ (for heterostructure with inclination axis about $[2\bar{1}\bar{1}0]$) and $\vartheta \sim 28°$ (for heterostructure with inclination axis about $[\bar{1}100]$); formation of MDs is impossible in such oriented heterostructures due to vanishing of ε_m because of the values of κ-Ga_2O_3 and α-Al_2O_3 crystal lattice parameters (see Eqs. (2)–(5) and Table 1). Second special case takes place at $\vartheta = 90°$; formation of MDs becomes impossible, because there is no component of MDs Burgers vector contributing to the energy release during relaxation process [20–22,25]. These facts suggest that the use of substrates oriented in a certain way, for example, the use of α-Al_2O_3 substrates with traditional (a-plane, m-plane) and exotic [$(10\bar{1}7)$, $(10\bar{1}6)$, $(2\bar{1}\bar{1}11)$, $(2\bar{1}\bar{1}9)$, etc.] growth planes, will make it possible to grow κ-Ga_2O_3 films with a low density of MDs.

As can be seen from Fig. 2, formation of pure edge MDs with $\boldsymbol{b}$[100] and $\boldsymbol{b}$[010] is energetically favorable (takes place at lower values of film thickness) than formation of mixed MDs with $\boldsymbol{b}$[110]. However, in the case of heterostructures with inclination axis about $[2\bar{1}\bar{1}0]$ crystallographic direction, the difference in thickness is insignificant (see Fig. 2a).

Due to similar crystal structure of κ-Al_2O_3 and κ-Ga_2O_3, we analyze dependences of the critical thickness h_c on the inclination angle ϑ for MDs formation in κ-$(Al_xGa_{1-x})_2O_3$/κ-Al_2O_3 heterostructures with various Al composition x; see Fig. 3. Solid, dashed and dash-dotted curves correspond to $x = 0$, 0.2, and 0.4, respectively. Analyzing these dependences, one can conclude that an increase in Al composition leads to an increase in the critical thickness for MDs formation. Despite the change in the Al composition, the formation of a pure edge MDs is energetically favorable than the formation of a mixed MDs in the considered heterostructures. Formation of pure edge MDs is easier in heterostructures with inclination axis about [010] crystallographic direction than in heterostructures with inclination axis about [100] crystallographic direction, and this is vice versa for mixed MDs.

4. CONCLUSIONS

The analytical model that describes critical conditions for pure edge and mixed MDs formation in film/substrate heterostructures with various growth orientations has been modified for κ-Ga_2O_3/α-Al_2O_3 and κ-$(Al_xGa_{1-x})_2O_3$/κ-Al_2O_3 heterostructures. Based on the symmetry of the crystal lattice of κ-Ga_2O_3, we consider two possibilities for variation in growth orientations of the film in κ-Ga_2O_3/α-Al_2O_3 and κ-Ga_2O_3/κ-Al_2O_3 heterostructures with inclination about either [100] or [010] crystallographic directions. Analytical expressions that describe the component of the lattice mismatch released by MDs have been proposed for heterostructures under consideration. It has been shown that for κ-Ga_2O_3/κ-Al_2O_3 heterostructures there are two special orientations, for which the formation of MD is unfavorable: (i) standard orientation at $\vartheta = 90°$, which is explained by the fact that there is no component of MDs Burgers vector contributing to the energy release during relaxation process; (ii) exotic orientation at $\vartheta \sim 26°$ (for heterostructure with inclination axis about [100] crystallographic direction of the film, or about $[2\bar{1}\bar{1}0]$ crystallographic direction of the substrate), and at $\vartheta \sim 28°$ (for heterostructure with inclination axis about [010] crystallographic direction of the film, or about $[\bar{1}100]$ crystallographic direction of the substrate) that is explained by vanishing of the component of the lattice mismatch released by MDs due to features of κ-Ga_2O_3 and α-Al_2O_3 crystal structure.

Calculations for κ-$(Al_xGa_{1-x})_2O_3$/κ-Al_2O_3 heterostructures have demonstrated that an increase in Al composition x leads to an increase in the critical thickness for MDs formation. Formation of mixed MDs is easier in heterostructures with inclination axis about [100] crystallographic direction than in heterostructures with inclination axis about [010] crystallographic direction, and this is vice versa for pure edge MDs.

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Релаксация напряжений за счет образования дислокаций в орторомбических пленках Ga_2O_3, полученных на подложках Al_2O_3

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Аннотация. Проанализирована предпочтительность образования различных типов дислокаций несоответствия (ДН) в гетероструктурах типа пленка/подложка κ-Ga_2O_3/α-Al_2O_3 и κ-$(Al_xGa_{1-x})_2O_3$/κ-Al_2O_3. Рассмотрены две возможные ориентации роста пленок, определяемые углом наклона ϑ, в упомянутых выше гетероструктурах с осями наклона относительно кристаллографических направлений [100] или [010]. Исследованы зависимости критической толщины пленки от угла наклона ϑ при зарождении ДН в рассматриваемых гетероструктурах. Установлено наличие двух особых ориентаций ($\vartheta \sim 26°$ для гетероструктуры [100], $\vartheta \sim 28°$ для гетероструктуры [010] и $\vartheta = 90°$ для обоих типов наклона) гетероструктур κ-Ga_2O_3/α-Al_2O_3, при которых образование ДН энергетически невыгодно. Показано, что в гетероструктурах [010] κ-$(Al_xGa_{1-x})_2O_3$/κ-Al_2O_3 образование краевых ДН предпочтительнее, чем в гетероструктурах [100], а для смешанных ДН – наоборот.

Ключевые слова: гетероструктуры типа пленка/подложка; оксид галлия; ориентация роста; дислокации несоответствия